# ATTACHMENT A

John McCray, Colorado Oil and Gas Conservation Commission

**Unnumbered in cover letter**

The DOE report demonstrates a high level of technical competence; the modeling work and analysis are technically sound. No obviously serious flaws were discovered in the analysis described in the report.

We thank the reviewer for sharing his observations in this regard.

**Unnumbered in cover letter**

However, I have identified some technical weaknesses that should be considered when evaluating the results in the report.

The main thrust of my analysis deals with whether or not the authors use acceptable conceptual models at various stages of the work. As an engineering analysis, the work is objective and rigorous within the constraints of the conceptual model used. However, the ultimate goal is to assess the risk of tritium reaching potential receptors. Risk assessment requires not only a sound technical analysis of a single conceptual model, but also an evaluation of several likely conceptual models. In this area, the DOE report is not as strong as it could be. In addition, while the Monte Carlo approach used is very rigorous given the available data, the available data may not justify using this approach. Finally, while uncertainty in the sub-surface away from the cavity is treated as rigorously as possible, the uncertainties in some other important model-input parameters are disregarded.

We agree with the reviewer on the importance of assessing conceptual model uncertainty for risk analysis, and our team has expertise assessing parametric and conceptual model uncertainty. For example, we assessed conceptual model uncertainty for another DOE project where alternative recharge models and alternative geological models exist at the Nevada Test Site. At the Rulison site, the conceptual model of the geologic system is well established as a result of intensive gas field development in the region, and we know of no reasonable alternatives to pose in contrast to the occurrence of fractured, discrete sand lenses. Ongoing exploration may identify other alternatives in the future. Currently, alternative conceptual models for this problem lie in the realm of proper mathematical description of flow and transport processes in a dual-phase fractured medium. Although multiple conceptual models can be postulated for features such as tortuosity, there is no solid support for the models, due not only to lack of data but also to lack of fundamental research. In other words, discrimination among alternative conceptual models (some of them may be wrong) is difficult. To deal with this problem, we adapted the principle of parsimony described in Neuman and Wierenga (2003, *A Comprehensive Strategy of Hydrogeologic Modeling and Uncertainty Analysis for Nuclear Facilities and Sites,* NUREG/CR-6805, U.S. Nuclear Regulatory Commission, Washington, D.C.) to postulate the conceptual model that can explain observed physical and chemical processes. Similarly, when choosing modeling techniques, we selected those commonly used in multiphase modeling and also believed appropriate at the Rulison site.

Responses to the comments on the Monte Carlo approach and other uncertainty parameters are given in detail below.

**Unnumbered in cover letter**

The problem, and thus the modeling effort and analyses, are very complex. Thus, please consider my attached findings preliminary. I would need more time to rigorously evaluate the identified technical weaknesses and to develop an opinion as to the impacts on the DOE report’s conclusions. For ease of digesting my findings, I have provided them as a numbered list in the attached pages.

**1.** The authors use an equivalent porous media (EPM) approach for evaluating tritium transport in fractured rock, a typical approach. However, for contaminant-transport modeling, this approach can have significant errors. Fracture flow modeling (which TOUGH2 is capable of) can be used to evaluate certain end-member cases. Because fracture data are not available (p.31 of the DOE report), it is likely that such an effort would yield highly uncertain results. Yet, an uncertainty analysis (similar to that used in the report) could be constructed and could lend considerable insight into contaminant transport behavior. Given the prevalence of fractures near the cavity, and the importance of fractures on solute transport, a dual-domain approach should be considered. This is especially true for this problem, where the physics of multiphase flow require that gas will flow in the larger fractures (fast flow pathway), and where partitioning of gas to the water phase (in the porous media) is the dominant mechanism for retardation.

We appreciate the reviewer's observations and agree that use of an EPM for fracture flow and transport is indeed an approximation of a complex system. Other workers (e.g., Snow 1968, 1969) demonstrated that many fracture-flow problems can be solved with standard porous-media techniques using Darcy's law and an anisotropic conductivity tensor. This avoids the many unsubstantiated assumptions needed to implement a discrete fracture model, as well as the theoretical problems associated with describing flow of fluids in fractures. Although TOUGH2 has a module capable of dual porosity/dual permeability flow and discrete fracture flow (we used this module in the earlier work for the Rio Blanco site), it is also based on Darcy's law, which rests on a continuum assumption.

When we compared the discrete fracture model to the EPM model on the Rio Blanco Project (Cooper et al. 2005, *Radionuclide Migration at the Rio Blanco Site, a Nuclear-Stimulated Low-Permeability Natural Gas Reservoir*, Desert Research Institute Rpt. No. 45215, DOE/NV/13609-45) we determined that for "typical" conditions at Rio Blanco, the medium could be considered homogeneous if the flow-controlling fractures were spaced 5 m apart, while it would need to be considered as heterogeneous for a fracture spacing of 20 m. Although those were idealized simulations, the formation properties between the two sites were similar, as the detonations were both done in the Mesaverde Group.

**2.** The partitioning of tritiated water vapor to the aqueous phase is the primary mechanism for contaminant retardation in this model, which increases travel times. While it is reasonable that this partitioning process is at equilibrium in the pore space, partitioning to water in the fractured zone, where the fractures are nearly dry, is limited by diffusion into the sandstone. This process could significantly reduce retardation in the fractured zone, and decrease travel times. In other words, the EPM approach results in instantaneous partitioning between the tritiated gas and water in the fracture zone, when partitioning in this zone may be diffusion limited and thus very small. Because of the EPM approach taken in the report, the potential importance of this effect was not evaluated.

Again, we understand the reviewer's concern regarding the EPM approach and its impact on important features such as the partitioning. However, it is not clear that equilibrium partitioning is an incorrect approximation. There are several factors here. One is the speed of equilibration itself. Experiments of tritium exchange (Slattery 1993) suggest isotopic equilibration times of about two seconds or less, and theoretical considerations show that it will depend on isotopic composition, surface area/volume ratio, and temperature. Equilibration can be expected to be rapid under subsurface conditions with the possible exception of very near the production well. Another factor is the diffusion into the sandstone to encounter liquid. The Williams Fork Formation has a liquid saturation of about 60 percent, such that there is ample water in the rock lining the fracture surfaces, suggesting that significant diffusion distances are not needed. Finally, as suggested by the reviewer, the fractures themselves may not be completely dry, nor create continuous pathways wholly discrete from the matrix. At these overburden pressures, with the low permeabilities indicated for these fractured rocks, and at these high water contents, the opportunity for contact between phases seems likely where fracture asperities may come into contact. (In addition, we know nothing about fracture aperture sizes at depths of 8000 ft.) Water may largely be in the matrix, but there is immediate contact between matrix and fractures (and the possibility of water films), as well as continuous gas phase between pores and fractures. Note that liquid is a known issue in the gas reservoir.

**3.** The relative permeability of the explosion-induced fracture zone is essentially equal to 1.0 because the gas will be flowing only in fractures, although in the EPM approach, it could be considerably less than this value (Figure 4-13).

We considered this while setting up the initial conditions; however, we determined that there could be liquid in the fractures for the following reasons: The fractures in question are not natural; they were created within the porous medium by the nuclear detonation. The condensation of steam occurred wherever water vapor was located, that is, in both the fractures and matrix. Over time, liquid water would diffuse from the fractures to the matrix, but this would almost certainly take from decades to perhaps thousands of years, depending upon the nature of the fracture coatings developed from the nuclear blast and the nature of the porosity and tortuosity associated with the porous medium. In other words, the development of fractures led to pressure transients between fractures and matrix that would equilibrate over an unknown length of time.

**4.** The authors use a rigorous Monte Carlo simulation approach to account for uncertainty in the location of interbedded sand and shale layers by simulating many possible heterogeneity structures using the two materials. This approach was interesting and insightful. The approach produces results that represent median, 5$^{th}$ percentile, and 95$^{th}$ percentile transport scenarios, which are highly useful with respect to decision making related to risk assessment. However, with only two conditioning points (wells RE and REX), I am not convinced the time and effort spent on this approach was commensurate with the information gained. The vertical information is useful, but only in a small area associated with the test site. Two points are not nearly sufficient to obtain meaningful horizontal information. I agree with the authors that the “overall poor continuity of sand lenses inhibits flow” in the modeled results (page 85). However, it is not known (based on the information in the report) whether or not this poor continuity is consistent throughout the site. If it is not, then the results could be influenced considerably. If the subsurface is similar in heterogeneity structure throughout the site, then this approach is appropriate and useful for risk assessment with respect to transport away from the cavity.

The heterogeneity of the Williams Fork is well characterized in the Piceance Basin. The poor continuity of sand lenses, determined in outcrop and through detailed well log analysis, is accepted for Williams Fork gas fields throughout the basin. This character is what has led to intense infill drilling on very close horizontal spacings.

A realistic depiction of the subsurface at Rulison needs to mimic the discrete, fluvial-deposited sand bodies. However, that architecture is complex and difficult to predict, even if there were many more conditioning points (contrast this to constructing a model of laterally continuous stratigraphy, for instance in a marine setting, where extrapolation can be done with more confidence). Since 500 realizations of the heterogeneous fields were generated, it is expected that randomness of the hydrofacies due to spatial variability is addressed and the characteristics of the subsurface heterogeneity reflected.

Two points is certainly not enough for the horizontal information, which instead came from the outcrop studies in Coal Canyon. The work of Cole and Cumella (2004; cited in the modeling report) is the basis of the spatial statistics, and we compared their observations to those from well-studied subsurface sites in the interior of the basin. It is likely that the horizontal continuity is somewhat exaggerated (which is more conservative, allowing higher probability of long transport distances) due to the orientation of outcrop exposures relative to strike.

**5.** Given the lack of data at the site, a more intuitive approach that considers simpler conceptual models of the subsurface may be useful to help decision makers evaluate risk. The geometries could take into account the dominant geologic features that are known to be consistent throughout the site. The "layer cake" simulation used in the non-isothermal simulations in the DOE report is a good example of this approach. The authors assumed a single sandstone layer connecting the production well and the cavity, and used a mean value for sandstone permeability and other properties. However, instead of using a mean value, various sources of information cited in the report could be used to obtain a limited distribution of permeability in the sandstone layer (supplementing it with other available data, if possible), and run simulation for median, quartile, and reasonable maximum and minimum values for permeability (and other variable, such as porosity). This approach would be useful in addition to the Monte Carlo analysis, and is an honest modeling effort in the face of limited data. Other "end-member" conceptual models could be tested using a similar approach.

We are not sure if we understand this comment correctly. The dominant geologic feature of the site is the interbedded sand and shale geometry, and distributions of permeability and porosity, based on data, were used for those parameters in the bulk of the work. A simplified domain was needed for the computationally intensive nonisothermal sensitivity analysis, but it is unclear how additional simulations of a nonrealistic layer-cake geometry would add information to the Monte Carlo analysis.

We agree that using a simplified domain allows for easier sensitivity testing of some model features. But this unrealistic simplification can lead to erroneous conclusions because it artificially eliminates the role of subsurface heterogeneity. We struggled with this in the sensitivity analyses presented in the report. For example, assuming a higher production rate may have a significant impact when continuous, high-permeability sands connect the chimney and pumping well but would have essentially no effect when shale blocks the connection. A sensitivity analysis using a continuous sand layer would conclude that production rate is a highly sensitive parameter, when in fact, the heterogeneous facies distribution determines its importance.

We agree with the reviewer that, given a lack of data, a simple model is preferred according to the principle of parsimony. However, we believe that the simple model should also be consistent with observed geological, physical, and chemical processes. With the known interlayered sandstone and shale structure prevalent at the site, a "layer cake" geological model does not appear appropriate.

**6.** The appropriateness of the high residual saturation used for the sandstone (0.5) should be evaluated more closely, particularly given that travel times are significantly influenced by gas-water partitioning. The data from Randolph (1983) suggest that saturations can be much smaller, which would reduce partitioning and significantly increase travel times.

Our understanding is that smaller liquid saturations would result in less partitioning from the gas to aqueous phase and lead to higher concentrations in the gas phase, which would *decrease* travel times.

Although Randolph (1983) measured initial liquid saturations as low as 22 percent, there are saturation values presented in his Table 1 as high as 95 percent, which could result in the opposite behavior. We used the mean saturation to smooth out the variations. The mean liquid saturation of Randolph's measurements presented is 49.6 percent.

**7.** Given the rigorous Monte Carlo approach used to evaluate uncertainty in subsurface heterogeneity away from the cavity, it in interesting the authors use a single-value deterministic approach for some other critically important model-input parameters. The intrinsic permeability of the explosion-related fractures is an important example. Published results from field experiments demonstrate that the permeability near the source of a contaminant can be a primary factor controlling the travel time of a contaminant to a downstream. The uncertainty in this parameter should be investigated. If the permeability of this zone is 100 times higher than the sandstone surrounding the fractured zone, which seems reasonable, then transport times could be considerably reduced. With the current distribution of permeability, this is likely to important for only the higher-percentile simulations. A similar comment could be made about the permeability of the nuclear chimney, although this permeability is considerably higher than that used in most simulations for the sandstone, so it would not decrease travel times. However, if other conceptual models are simulated in the future, then it may be important to evaluate lower permeabilities (as well as higher potential values) for the nuclear chimney and the zone of explosion-related fractures to obtain a distribution of travel times. Another factor in this category is the relative permeability, which is described below.

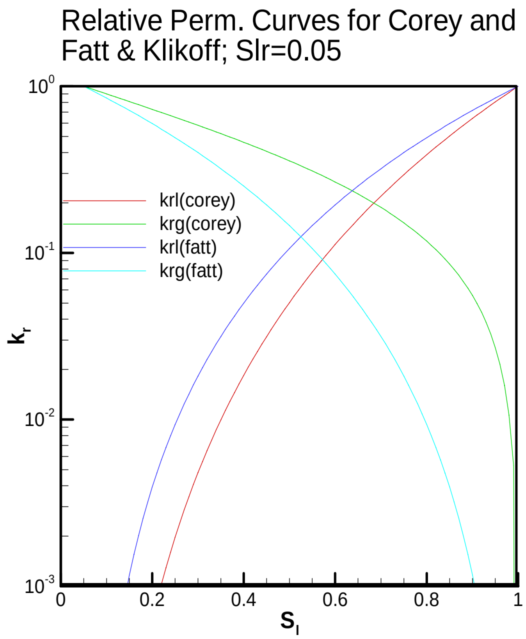
The permeability of the nuclear-fracture zone was not treated as a random parameter in the model because two independent analyses of production from the nuclear chimney resulted in similar values. In other words, site-specific data supported that the value was $3 \times 10^{-16}$ $m^2$ or less. Lower values were also obtained and could have been used to develop a distribution, but that was not as conservative a choice as setting the permeability at the highest measured value. In contrast, the permeability of the chimney itself is inferred, but as the reviewer notes, it is very high and is indeed higher than all of the simulations of the sandstone. We appreciate the fact that the reviewer recognizes that lower permeabilities are also possible.

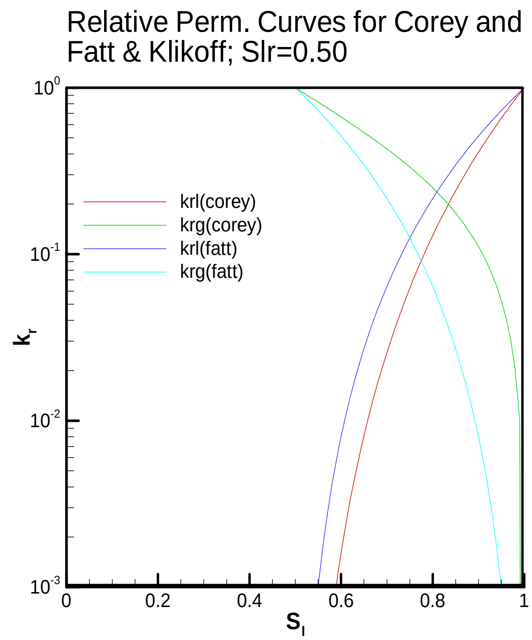
Note that due to rapid diffusion in the gas phase, tritium readily migrates throughout the nuclear chimney and nuclear-fracture zone, extending to the edge of the fracture zone within the 38 years of pre-production.

Given the site-specific data, there is no justification for arbitrarily increasing the nuclear-fracture zone permeability by orders of magnitude. However, during discussions with COGCC personnel at a meeting on November 8, 2007, James Adkins suggested additional evaluation of the Rulison production testing data. If the original data can be found, we will evaluate them in the context of the reviewer's comment.

**8.** The relative permeability function induce considerable uncertainty into the model via several avenues that is not considered in the analysis. First, the relationship between relative permeability and water content can vary considerably depending on the relationship used. The current model uses only the Corey (1954) relationship without verification. Other relationships (e.g., Stone, Fatt and Klickoff, etc) could result in relative permeabilities that are considerably different for the same water content.

It is correct that we did not look at uncertainty in the choice of relative permeability functions. We determined that the uncertainty due to the function was well within the uncertainty in the permeability field. For example, attached at the end of the document is a plot of the relative permeability curves of Corey and Fatt & Klikoff for each of the gas and liquid phases. For a residual liquid saturation of 0.5, (the situation for our simulations; the lower plot), the curves are remarkably similar. Although operationally defined, the relative permeability to gas curves are very similar at $S_l = 0.5$, which is the liquid saturation value throughout most of the domain for most simulations.




**9.** The relative permeability function used is not consistent with the data from Randolph (1983). This results primarily from the higher residual saturation (equal to 0.5) used in this model. If a very small residual saturation is used, then the curves used would be consistent with the data.

We alluded to this inconsistency on page 49 of the report. Some of Randolphs's measurements were made at saturations below what was defined as residual saturation. His measurements were made with mercury, which allowed measurements at lower moisture contents, which could not occur in the field except at very low saturations. We honored Randolph's data from full liquid saturation (i.e., $S_l$ = 1) to the residual value, $S_{lr}$ = 0.5.

**10.** Additional simulations investigating the impact of fully screened wells, or additional wells could be useful. The bulk of the authors analysis assume that the production well is screened only at the level of the contaminant source, and is extracting at 1/10$^{th}$ of the rate of a typical well. This is presumed to lead to an underestimate of contaminant travel times. However, given the highly discontinuous and vertically heterogeneous mature of the subsurface, a single well extracting at a higher rate over a large depth interval could draw contaminant vapor to locations higher in the subsurface that are not captured by the well (and thus available for upward diffusion). It is difficult to say if this process is important without additional simulations.

The production scenario is entirely hypothetical, and any number of other conditions could be investigated. For example, of great importance is the actual x-y location of the well.

It is true that there can be vertical connections between sand lenses such that a longer screen or multiple, screens could result in more overall mass movement to the well. However, the highest concentration should be realized through a single pathway, as simulated here. Of course, increasing the production rate will increase transport for a given interval, and is another hypothetical assumption.

**11.** There is a growing body of literature that suggests the advective-diffusive approach used in this work may significantly underestimate gas transport in fractured rock, especially when partitioning to the matrix is important. The Dusty Gas Model is thought to be a more appropriate approach, and I believe this has been incorporated into the TOUGH model, but perhaps not into a commercially available package. Nonetheless, the possibility that the approach used could overestimate travel times should be acknowledged.

The dusty gas model (DGM) is attractive in multicomponent mixtures in which none of the gases are in trace amounts. (The reason is that in, for example, binary systems with non-trace amounts of gases, diffusion of one gas results in the development of a concentration of the other gas in the opposite direction. Transport of each gas then becomes coupled to the other as the concentration field of one gas becomes dependent upon the properties of the other gas. This feature is not considered in the conventional advection-diffusion model [ADM].) Since our system deals with trace amounts of tritium (less than parts per billion), this feature may not be as important because a trace gas diffusing through a system will negligibly alter the concentration of the other gas.

Oldenburg et al. (2004, *Transport in Porous Media*, 54(3): 323–334) compared simulations of$CO_2$ and methane mixtures to investigate the suitability of the DGM as compared to the ADM. For their simulations, the DGM is recommended for low intrinsic permeability and very low pressure, while the ADM is recommended for higher permeability and/or high pressure. Their pressures did not exceed 4 MPa; our highest pressures are 20 MPa. Without testing the two models for our specific conditions, it seems that the ADM may still be appropriate for our situation. It is true that there exists a modification to the TOUGH2 code for the DGM.

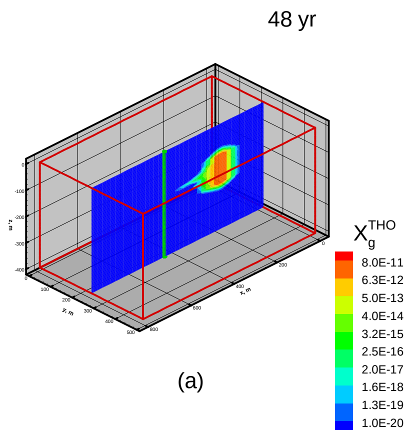
**12.** The Millington-quirk model used to estimate tortuosity, which controls diffusion, is not developed for fractured rock. The impacts of this assumption are not clear. In addition, even for porous media, the model is highly uncertain without calibration to data. Other means to estimate tortuosity could be evaluated to see if they would result in significantly different diffusion rates. In the current conceptual model, the diffusion is only important before and after operation of the production well (advection will dominate). However, diffusion of tritiated gas into the sandstone from fractures is likely very important feature at the site.

We explored the impact of using a relative permeability based model, instead of Millington-Quirk, in the Rio Blanco modeling. The relative permeability model enhances transport in both phases, but not to a large degree. A comparison of the Millington-Quirk and a relative permeability-based model (see the TOUGH2 user's Manual) resulted in very small differences for the Rulison permeability/porosity field that resulted in the 78$^{th}$ percentile breakthrough. (This was the only perm./porosity field tested.) The maximum extent of transport at a given time was nearly the same; however, the shape of the tritium mass fraction field differed between the two models at equivalent times. These results are shown in figures attached to this document. Without any peer reviewed acceptance of a relative permeability model, it did not seem appropriate as the primary basis of the Rulison work. The most commonly implemented model of tortuosity is the Millington-Quirk that includes phase-dependent saturation, and that is why it was selected for Rulison. Most models of tortuosity are based on research conducted in the late 1950s and 1960s. Additional research in regard to tortuosity in two phase systems, particularly fracture systems, is needed.

The last statement in this comment is essentially another retarding process. Diffusion from fractures into matrix blocks is indeed an important process slowing contaminant transport in fractured environments. Even in EPM approximations, some mass transfer function simulating matrix diffusion is often used (e.g., Liu et al., 2000 and follow-on developments such as Huang et al., 2003). Adding that process to the Rulison model would reduce contaminant migration.

millington-quirk saturation-based tortuosity model

relative permeability tortuosity model

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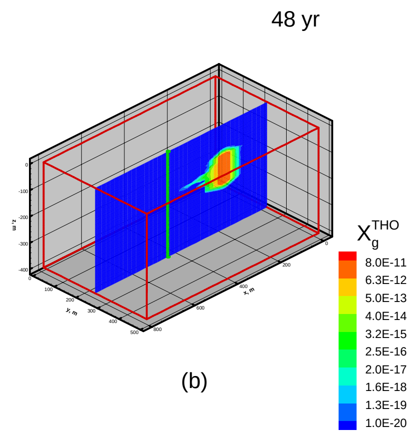


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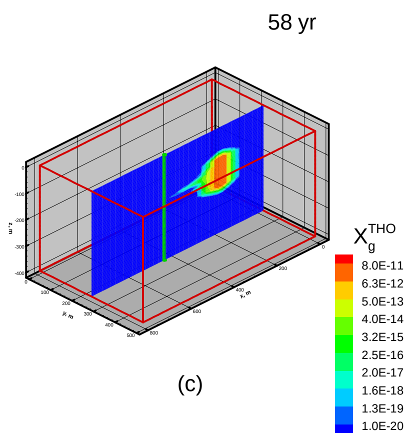


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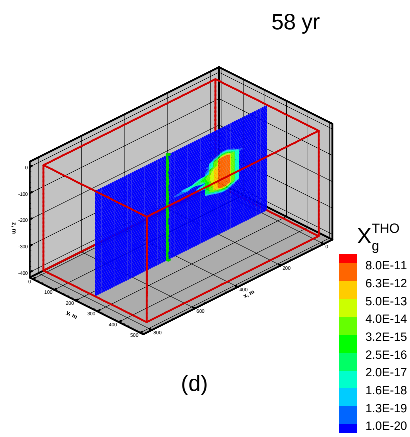


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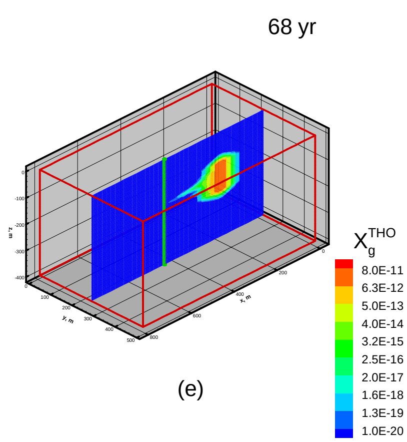


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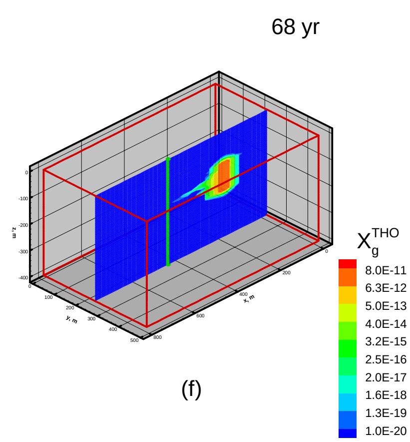


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millington-quirktortuosity model

relative-permeability-based tortuosity model

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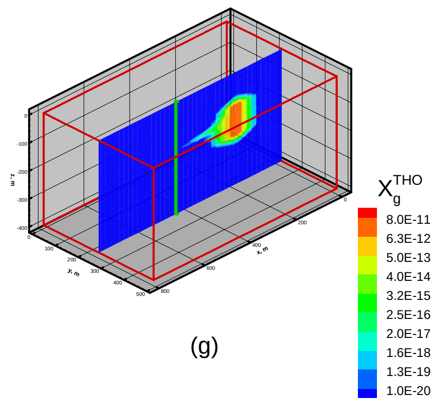


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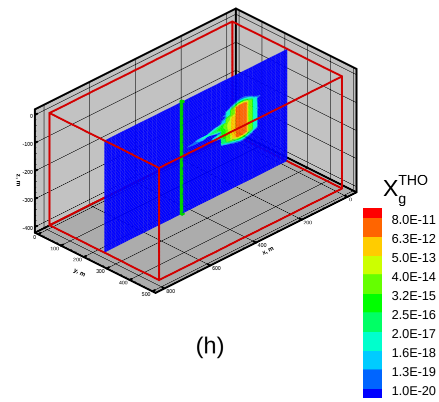
75 yr

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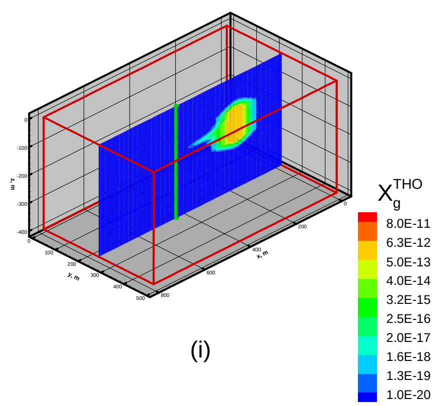
100 yr

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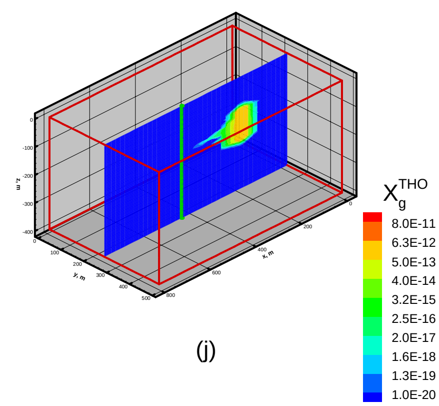


(j)

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**13.** The shales are assumed to be tight and continuous. If they are actually fractured, then the effective permeability of the subsurface could be much higher because the shales likely have a significant impact on the overall permeability in the current modeling approach.

The shales definitely have a significant impact in terms of continuity of permeable pathways. All of the information reviewed indicates that they are very impermeable and that fractures terminate at the shale contacts. Anecdotal discussions have suggested that hydrofractures may dynamically penetrate shales, but rapidly heal and seal. The behavior of the reservoir as discrete sand packages, consistent with the current intensive development, supports the shales as barriers between the sand lenses.

**14.** Strictly speaking, the TOUGH2 model is not designed for this problem. However, I am not aware of a model that is completely appropriate for simulating the tritium transport during natural gas production. The TOUGH2 model is not designed to handle this problem either. However, the authors have done a good job using the model's current capabilities to simulate the problem at hand. The arera that is not discussed sufficiently in the report is the use of water-air steam tables to obtain thermodynamic and volatilization properties for this methane-water system.

True, we assumed that the thermodynamic properties of air and methane were the same. This would affect phase exchange, which doesn't really occur in the simulations (except for a few noted in the Alternative Scenarios section) as they were isothermal. However, adjustments were made to the code in the equation of state such that gas densities and viscosities would be correct. This is discussed on page 39. We think that because both methane and air are noncondensable, their thermodynamic properties—pertaining to the steam tables—are not as important, for example, as modeling the phase exchange of tritiated water, which is thoroughly discussed on pages 51–54.